

Artificial Odor Cluster Map of Odorant Molecular Parameters and Odor Maps in Rat Olfactory Bulbs

Liang Shang¹, Chuanjun Liu², Yoichi Tomiura¹, Kenshi Hayashi^{1*}

¹Department of Electronics, Graduate School of Information Science and Electrical Engineering, Kyushu University

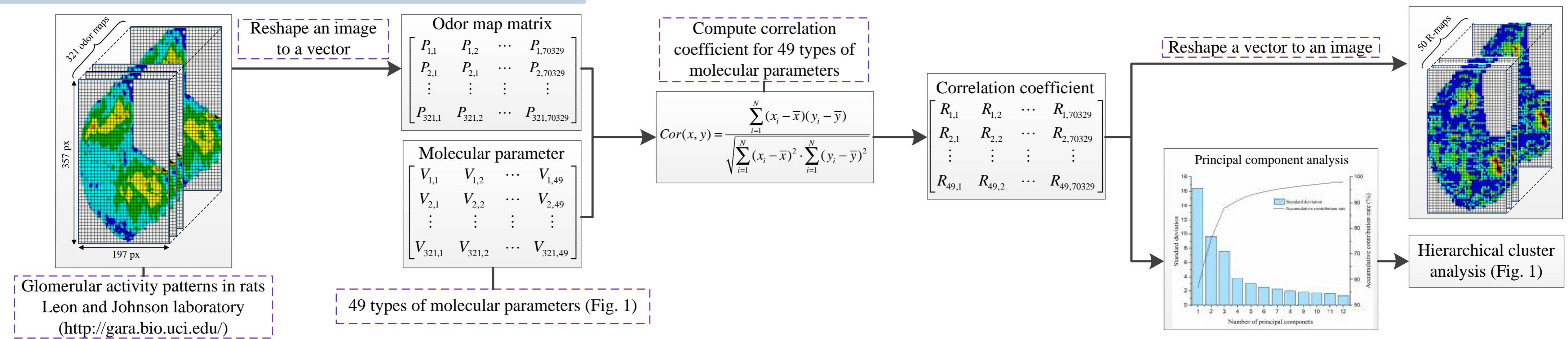
²Division of Odor Sensor, Research and Development Center for Taste and Odor Sensing, Kyushu University

HIGH LIGHT

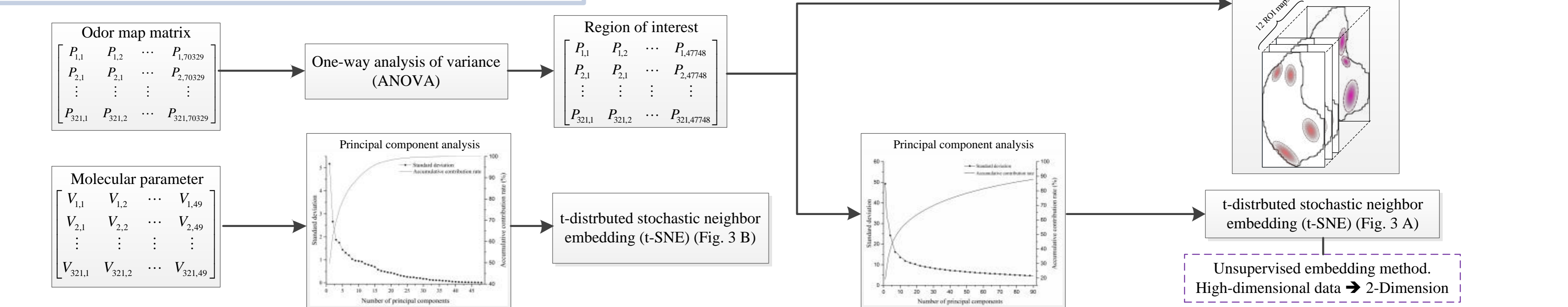
- Olfactory, as one of the most primitive sense, plays an essential role in mammals' daily life.
- To understand the mechanism of discriminating odorants by olfactory system is meaningful for developing odor sensors.
- 321 odor maps in rat olfactory bulbs and 49 types of molecular parameters were analyzed.
- Combined with PCA and t-SNE method, an artificial odor cluster map was established based on odor maps.

MATERIAL AND METHOD

R-maps for molecular features

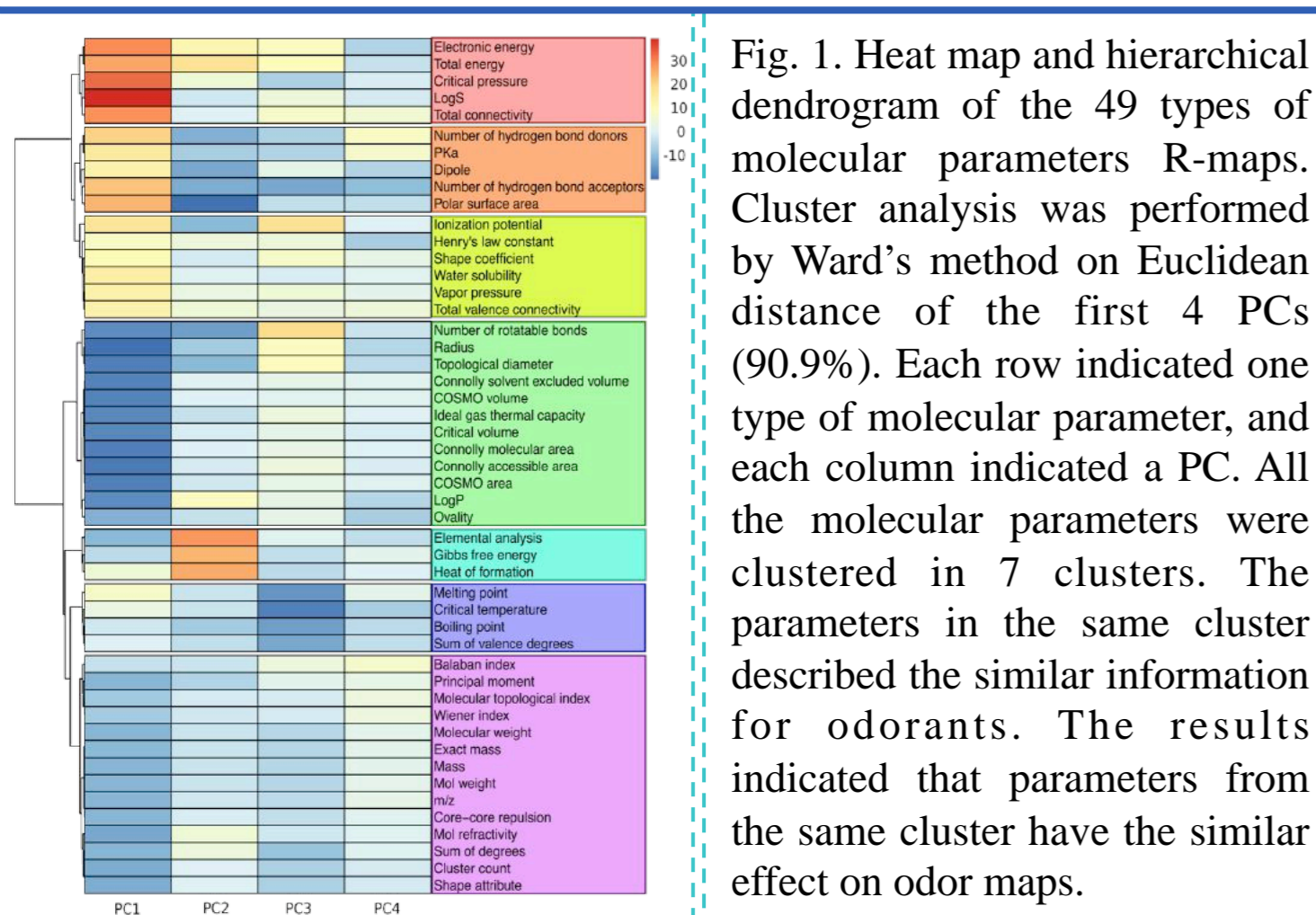


Mapping the odorants in a t-SNE space

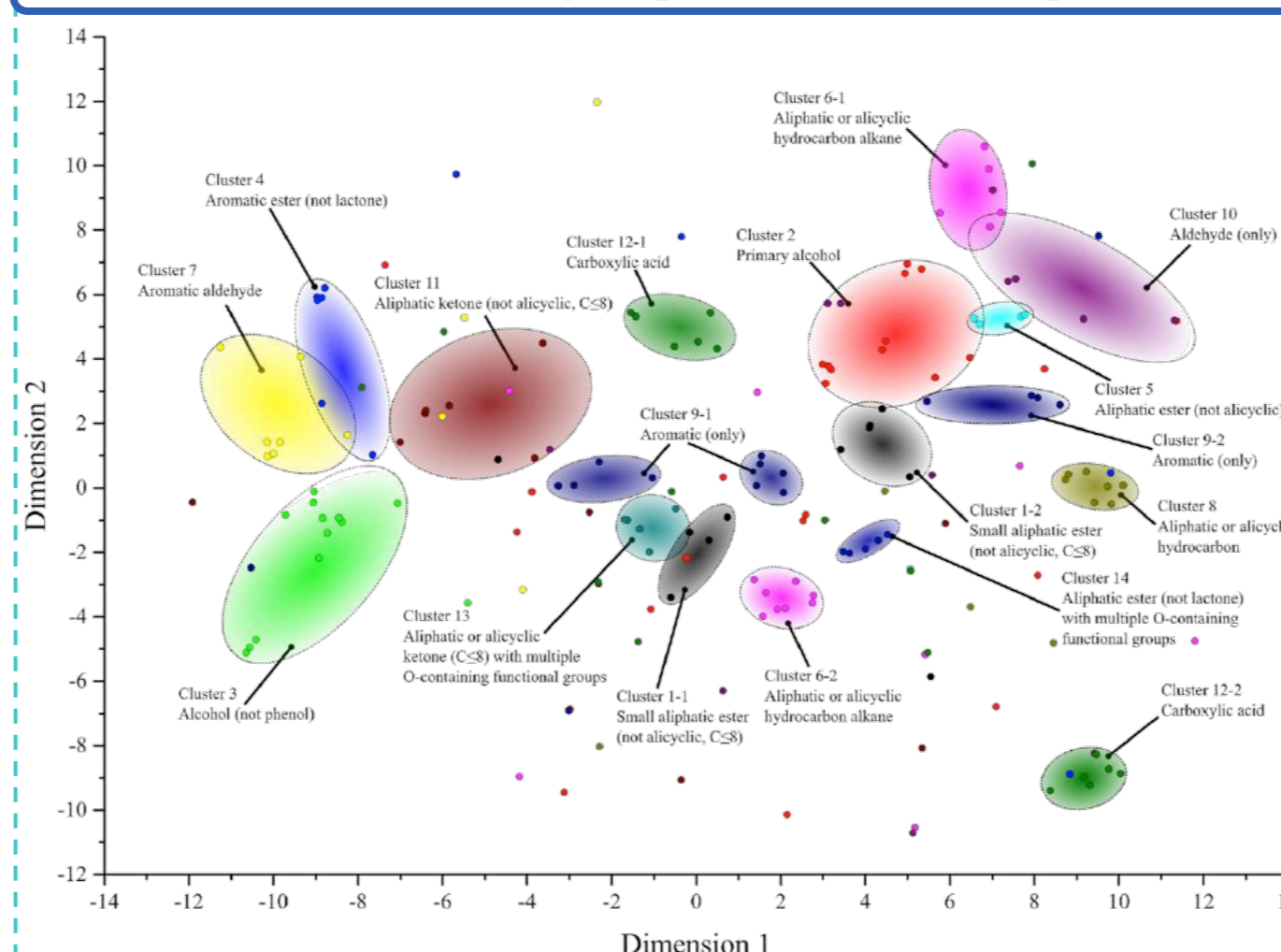


RESULTS AND DISCUSSION

Heat map and hierarchical dendrogram for molecular parameters



A. 2D embedding map based on odor maps



B. 2D embedding map based on molecular parameters

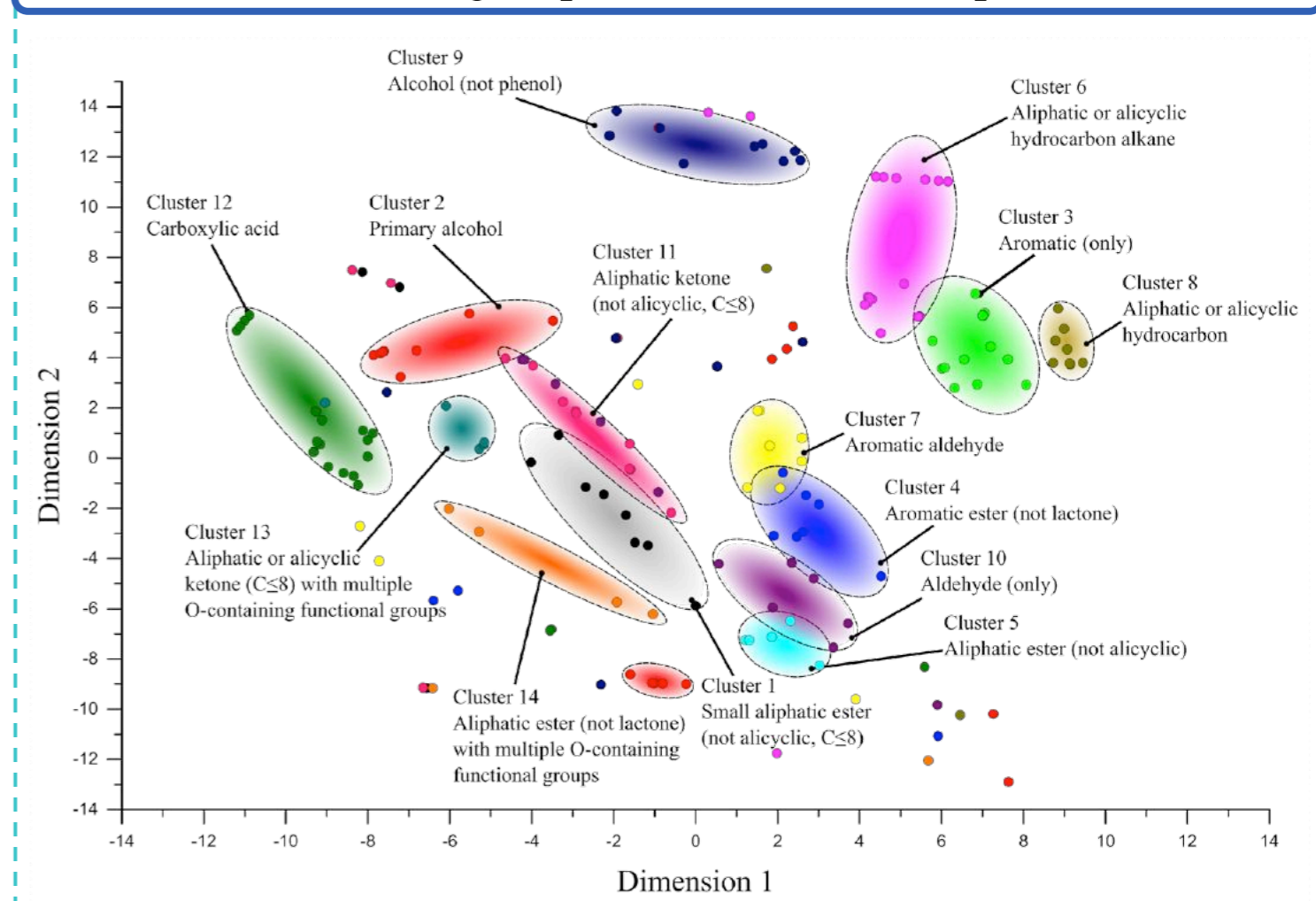


Fig. 3. 2D artificial cluster maps for 14 types of function group descriptions by t-SNE method. In the space established by odor maps (A), odorants with the same label are mostly clustered in one or two groups, respectively. However, some samples were not clustered in a group. Besides, some clusters are overlapped in the t-SNE map. In the space established by molecular parameters (B), more overlapped were observed. Some information could not be included in that map. The results indicated that an odorant could not be completely described only by molecular parameters.

CONCLUSIONS

- The relationship between molecular features of odorants and odor maps were discussed.
- Correlation maps for 49 types of molecular parameters can be clustered in 7 groups.
- Response regions for 12 types of main functional groups were extracted and evaluated.
- Odor maps combined with PCA and t-SNE method can be successfully utilized for mapping odorants in a 2D artificial cluster map.
- Compared with the artificial clustering map established by molecular parameters, that established by odor maps contained more information for odorants.
- This study would provide a technical basis for developing sensor-based machine olfaction.

Response regions for 12 types of functional groups

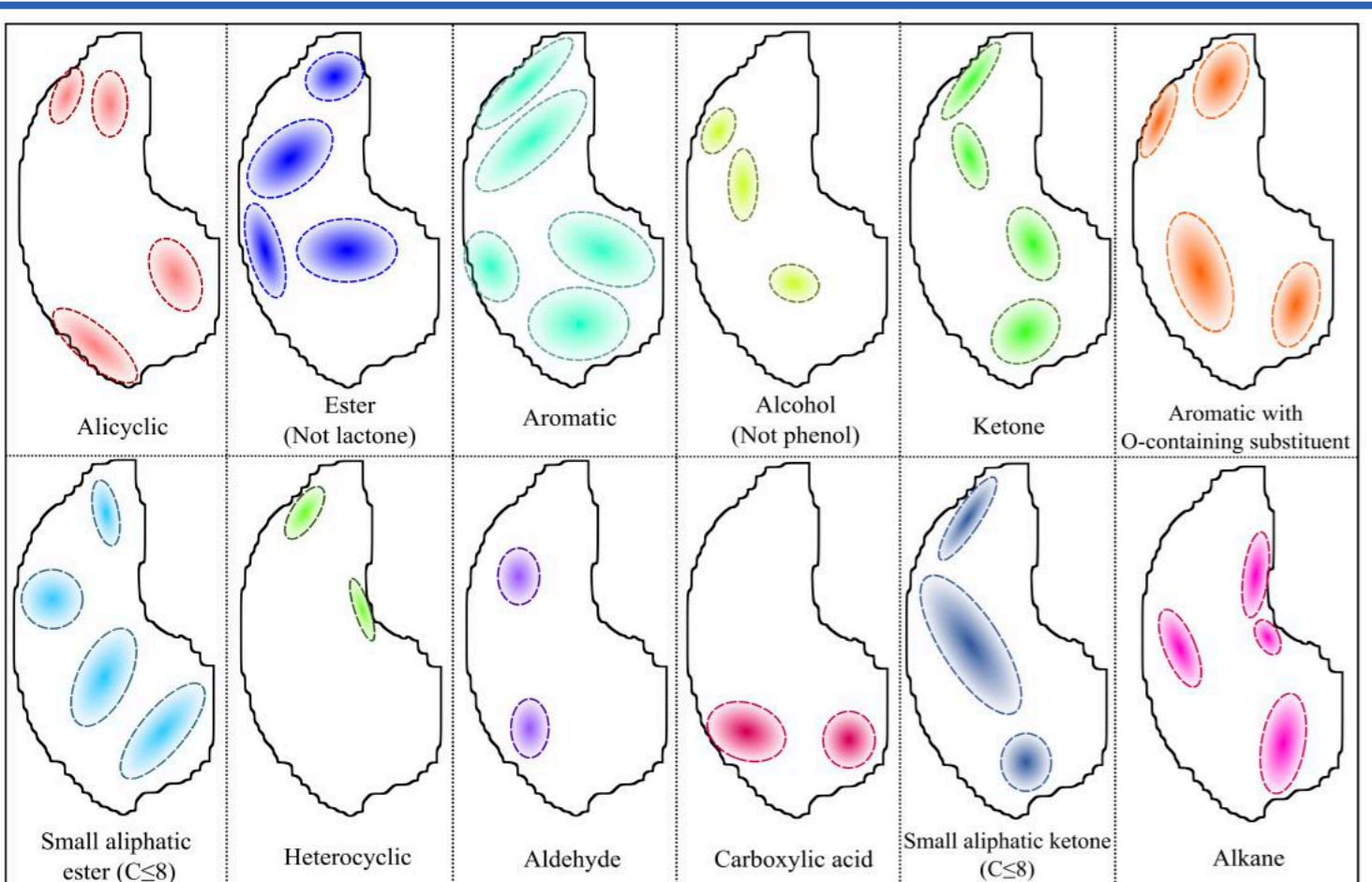


Fig. 2. Response regions for 12 types of functional descriptions are extracted by one-way analysis of variance (ANOVA). We can find some overlapped response regions were found by different functional descriptions.